AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions, and listings, of claims in the application.

Listing of Claims:

1-18. (cancelled).

19.   (currently amended) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, wherein the chemical entities comprise a phosphate residue or a surrogate for a phosphate residue; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

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a)   utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

b)   docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c)   analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

d)   optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e)   selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

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20.   (currently amended) A method of using a
computer for selecting at least one of a plurality of
chemical entities based on its ability to associate with
all or part of a molecule or molecular complex comprising a
CnA binding pocket defined by structure coordinates of CnA
amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156,
160, 199, 281, 282, 283, 306, 311, 232, and 254 according
to Figure 1, or a CnA homologue binding pocket that has a
root mean square deviation from the backbone atoms of said
amino acids of not more than 1.5Å, wherein the chemical
entities comprise a phosphate residue or a surrogate for a
phosphate residue;

wherein said computer comprises a machine-readable data
storage medium comprising a data storage material encoded
with said structure coordinates defining all or part of
said binding pocket and wherein said method comprises the
steps of:

        a)   utilizing said structure coordinates
defining all or part of said binding pocket and the
structure coordinates of one of said plurality of chemical
entities to position a chemical entity within all or part
of the CnA binding pocket or the CnA homologue binding
pocket;

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b)   docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c)   analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

d)   optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e)   selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

21.   (currently amended) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a <u>molecule or molecular complex comprising a</u> CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314,

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339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å, wherein the chemical entities comprise a hydrophobic core and a 10-14 Å linker that projects a hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 115, 118 and 119 of CnB and amino acid residues 352, 353, 356 and 357 of CnA according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a)   utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part

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of the CnA/CnB binding pocket or the CnA/CnB homologue
binding pocket;

      b)   docking said chemical entity and the
CnA/CnB binding pocket or the CnA/CnB homologue binding
pocket by employing computational means which utilize said
structure coordinates of all or part of the binding pocket
or the chemical entity wherein said docking utilizes energy
minimization;

      c)   analyzing the results of said docking
to quantify the association between said chemical entity
and all or part of the CnA/CnB binding pocket or the
CnA/CnB homologue binding pocket;

      d)   optionally repeating steps a) through
c) with another of said plurality of chemical entities; and

      e)   selecting at least one of said
plurality of chemical entities that associates with all or
part of the CnA/CnB binding pocket or the CnA/CnB homologue
binding pocket based on said quantified association of said
chemical entity.

    22.   (currently amended) A method of using a
computer for selecting at least one of a plurality of
chemical entities based on its ability to associate with
all or part of a molecule or molecular complex comprising a

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binding pocket defined by CnA amino acids 90, 91, 92, 118,

120, 121, 122, 124, 150, 151, 156, 159, 160, 199, 232, 253,

254, 256, 281, 282, 283, 284, 306, 310, 311, 312, 313, 314,

317, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355,

356, 359, 360, and 363; and CnB amino acids 49, 50, 114,

115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and

162 according to Figure 1, or a homologue binding pocket

that has a root mean square deviation from the backbone

atoms of said CnA and CnB amino acids of not more than

1.5Å, wherein the chemical entities comprise a hydrophobic

core and a 10-14 Å linker that projects a hydrophobic

moiety from the center of the hydrophobic core to make a

Van der Waals contact with all or part of amino acid

residues 115, 118 and 119 of CnB and amino acid residues

352, 353, 356 and 357 of CnA according to Figure 1, or

amino acids of a CnA/CnB homologue that have a root mean

square deviation from the backbone atoms of said CnA and

CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data

storage medium comprising a data storage material encoded

with said structure coordinates defining all or part of

said binding pocket and wherein said method comprises the

steps of:

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a)   utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b)   docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c)   analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

d)   optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e)   selecting at least one of said plurality of chemical entities that associate with all or part of the CnA/CnB binding pocket or CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

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23.   (currently amended) A method for using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex defined by the entire set of structure coordinates of CnA/CnB amino acids according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å, wherein the chemical entities comprise a hydrophobic core and a 10-14 Å linker that projects a hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 115, 118 and 119 of CnB and amino acid residues 352, 353, 356 and 357 of CnA according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said molecule, molecular complex, or homologue thereof and wherein said method comprises the steps of:

a)   utilizing said structure coordinates defining all or part of said molecule, molecular complex,

or homologue thereof and the structure coordinates of one

of said plurality of chemical entities to position a

chemical entity within all or part of the molecule,

molecular complex, or homologue thereof;

b)   docking said chemical entity with all or

part of the molecule, molecular complex, or homologue

thereof by employing computational means which utilize said

structure coordinates of all or part of the molecule,

molecular complex, or homologue thereof or the chemical

entity, wherein said docking utilizes energy minimization;

c)   analyzing the results of said docking to

quantify the association between said chemical entity and

all or part of the molecule, molecular complex, or

homologue thereof;

d)   optionally repeating steps a) through c)

with another of said plurality of chemical entities; and

e)   selecting at least one of said plurality of

chemical entities that associate with all or part of the

molecule, molecular complex, or homologue thereof based on

said quantified association of said chemical entity.

24.   (previously presented) The method according

to claim 23, wherein said molecular complex is defined by

the structure coordinates of the amino acids of CnA, the

amino acids of CnB, FKBP12 and FK506 according to Figure 1,
or a homologue thereof, wherein said homologue has a root
mean square deviation from the backbone atoms of said CnA
and CnB amino acids of not more than 1.5 Å.

          25.   (currently amended) A The method according
to any one of claims 19-24, for identifying a compound
capable of associating with a molecule comprising a CnA-
like binding pocket further comprising the steps of:

          a.   using the atomic coordinates of CnA amino
acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160,
199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312,
and 317 according to Figure 1 : a root means square
deviation from the backbone atoms of said amino acids of
not more than 1.5 Å, to generate a three dimensional
structure of a molecule comprising a CnA-like binding
pocket;

          b.   employing said three dimensional structure
to design or select said compound;

          c.   synthesizing said compound; and

          [[d.]] f) contacting the selected chemical entity
said compound with said molecule or molecular complex to
determine the ability of said compound to interact with
said molecule; and

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g)   monitoring the association of the molecule or molecular complex with the selected chemical entity.

26-30. (cancelled).

31.   (previously presented) The method according to any one of claims 19, 20, 21 and 22, wherein prior to step a), further comprising the steps of:

a)   producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b)   determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

c)   identifying all or part of said binding pocket.

32.   (currently amended) The method according to any one of claims 25, 26 and 27, claim 23, wherein prior to step a), further comprising the steps of:

a)   producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

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b)   determining the three-dimensional
structure coordinates of the molecule or molecular complex
by X-ray diffraction of the crystal, and

~~c)   identifying all or part of said binding
pocket.~~

33.   (currently amended) The method according to
any one of claims 19, 20 ~~and~~, 21, 22 and 23 wherein the
docking utilizes shape complementarity or is followed by
molecular dynamics.

34.   (currently amended) The method according to
any one of claims 19, 20 ~~and~~, 21, 22 and 23 wherein the
docking is performed through visual inspection on a
computer screen using a computer program capable of
generating a three-dimensional graphical representation of
said structure coordinates and structure coordinates of
said chemical entity.

35.   (new)   The method according to any one of
claims 19-22, further comprising the steps of:

f)   repeating steps a) to e) with a second set
of a plurality of chemical entities that associate with all
or another part of the binding pocket or homologue thereof;

g)   optionally, visually inspecting the
relationship of the selected first and second chemical
entity to each other in relation to the binding pocket or
homologue thereof on a computer screen using the three-
dimensional graphical representation of the binding pocket
or homologue thereof and said selected first and second
chemical entity; and

h)   assembling the selected first and second
chemical entity into a compound or complex that associates
with all or part of said binding pocket or homologue
thereof by model building.

36.   (new) The method according to claim 23 or
24, further comprising the steps of:

f)   repeating steps a) to e) with a second set
of a plurality of chemical entities that associate with all
or another part of the molecule or molecular complex or
homologue thereof;

g)   optionally, visually inspecting the
relationship of the selected first and second chemical
entity to each other in relation to the molecule or

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molecular complex or homologue thereof on a computer screen

using the three-dimensional graphical representation of the

molecule or molecular complex or homologue thereof and said

selected first and second chemical entity; and

h)   assembling the selected first and second

chemical entity into a compound or complex that associates

with all or part of said molecule or molecular complex, or

homologue thereof by model building.

37.   (new) A method of using a computer for

selecting at least one of a plurality of chemical entities

based on its ability to associate with all or part of a

molecule or molecular complex comprising a calcineurin A

(CnA) binding pocket defined by structure coordinates of

CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151,

156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306,

311, 312, and 317 according to Figure 1, or a CnA homologue

binding pocket that has a root mean square deviation from

the backbone atoms of said amino acids of not more than

1.5Å;

wherein said computer comprises a machine-readable data

storage medium comprising a data storage material encoded

with said structure coordinates defining all or part of

said binding pocket and wherein said method comprises the steps of:

a)   producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b)   determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c)   identifying all or part of said binding pocket;

d)   utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

e)   docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f)   analyzing the results of said docking to quantify the association between said chemical entity

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and all or part of the CnA binding pocket or the CnA
homologue binding pocket;

      g) optionally repeating steps a) through
c) with another of said plurality of chemical entities; and

      h) selecting at least one of said
plurality of chemical entities that associates with all or
part of the CnA binding pocket or the CnA homologue binding
pocket based on said quantified association of said
chemical entity.

    38. (new) A method of using a computer for
selecting at least one of a plurality of chemical entities
based on its ability to associate with all or part of a
molecule or molecular complex comprising a calcineurin A
(CnA) binding pocket defined by structure coordinates of
CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151,
156, 160, 199, 281, 282, 283, 306, 311, 232, and 254
according to Figure 1, or a CnA homologue binding pocket
that has a root mean square deviation from the backbone
atoms of said amino acids of not more than 1.5Å;
wherein said computer comprises a machine-readable data
storage medium comprising a data storage material encoded
with said structure coordinates defining all or part of

said binding pocket and wherein said method comprises the steps of:

a)   producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b)   determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c)   identifying all or part of said binding pocket;

d)   utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

e)   docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f)   analyzing the results of said docking to quantify the association between said chemical entity

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and all or part of the CnA binding pocket or the CnA

homologue binding pocket;

g)   optionally repeating steps d) through

f) with another of said plurality of chemical entities; and

h)   selecting at least one of said

plurality of chemical entities that associates with all or

part of the CnA binding pocket or the CnA homologue binding

pocket based on said quantified association of said

chemical entity.

39.   (new) A method of using a computer for

selecting at least one of a plurality of chemical entities

based on its ability to associate with all or part of a

molecule or molecular complex comprising a CnA/CnB binding

pocket defined by structure coordinates of CnA amino acids

122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344,

345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363;

and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118,

119, 121, 122, 123, 124, 157, 158, 159, 161, and 162

according to Figure 1, or a CnA/CnB homologue binding

pocket that has a root mean square deviation from the

backbone atoms of said CnA and CnB amino acids of not more

than 1.5Å;

wherein said computer comprises a machine-readable data

storage medium comprising a data storage material encoded

with said structure coordinates defining all or part of

said binding pocket and wherein said method comprises the

steps of:

    a)   producing a crystal of a molecule or

molecular complex comprising amino acids 5-168 of CnA and

amino acids 24-370 of CnB and a chemical entity;

    b)   determining the three-dimensional

structure coordinates of the molecule or molecular complex

by X-ray diffraction of the crystal;

    c)   identifying all or part of said binding

pocket;

    d)   utilizing said structure coordinates

defining all or part of said binding pocket and the

structure coordinates of one of said plurality of chemical

entities to position a chemical entity within all or part

of the CnA/CnB binding pocket or the CnA/CnB homologue

binding pocket;

    e)   docking said chemical entity with all

or part of the CnA/CnB binding pocket or the CnA/CnB

homologue binding pocket by employing computational means

which utilize said structure coordinates of all or part of

the binding pocket or the chemical entity, wherein said

docking utilizes energy minimization;

f)   analyzing the results of said docking

to quantify the association between said chemical entity

and all or part of the CnA/CnB binding pocket or the

CnA/CnB homologue binding pocket;

g)   optionally repeating steps d) through

f) with another of said plurality of chemical entities; and

h)   selecting at least one of said

plurality of chemical entities that associates with all or

part of the CnA/CnB binding pocket or the CnA/CnB homologue

binding pocket based on said quantified association of said

chemical entity.

40.   (new) A method of using a computer for

selecting at least one of a plurality of chemical entities

based on its ability to associate with all or part of a

molecule or molecular complex comprising a CnA/CnB binding

pocket defined by structure coordinates of CnA amino acids

90, 91, 92, 118, 120, 121, 122, 124, 150, 151, 156, 159,

160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 310,

311, 312, 313, 314, 317, 339, 341, 343, 344, 345, 347, 351,

352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino

acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157,

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158, 159, 161, and 162 according to Figure 1, or a CnA/CnB

homologue binding pocket that has a root mean square

deviation from the backbone atoms of said CnA and CnB amino

acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data

storage medium comprising a data storage material encoded

with said structure coordinates defining all or part of

said binding pocket and wherein said method comprises the

steps of:

a)   producing a crystal of a molecule or

molecular complex comprising amino acids 5-168 of CnA and

amino acids 24-370 of CnB and a chemical entity;

b)   determining the three-dimensional

structure coordinates of the molecule or molecular complex

by X-ray diffraction of the crystal;

c)   identifying all or part of said binding

pocket;

d)   utilizing said structure coordinates

defining all or part of said binding pocket and the

structure coordinates of one of said plurality of chemical

entities to position a chemical entity within all or part

of the CnA/CnB binding pocket or the CnA/CnB homologue

binding pocket;

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e) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

g) optionally repeating steps d) through f) with another of said plurality of chemical entities; and

h) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

41. (new) The method according to any one of claims 37-40, further comprising the steps of:

i) contacting the selected chemical entity with said molecule or molecular complex; and

j) monitoring the association of the molecule or molecular complex with the selected chemical entity.

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42.   (new) The method according to any one of claims 37-40, wherein the docking utilizes shape complementarity or is followed by molecular dynamics.

43.   (new) The method according to any one of claims 37-40, wherein the docking is performed through visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.

44.   (new) The method according to any one of claims 37-40, further comprising the steps of:

i)   repeating steps d) to h) with a second set of a plurality of chemical entities that associate with all or another part of the binding pocket or homologue thereof;

j)   optionally, visually inspecting the relationship of the selected first and second chemical entities to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

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k)   assembling the first and second chemical

entities into a compound or complex that associates with

all or part of said binding pocket or homologue thereof by

model building.

45.   (new) The method according to any one of

claims 21-24, wherein the chemical entities further

comprise a linker of 7-11 Å that projects a second

hydrophobic moiety from the center of the hydrophobic core

to make a Van der Waals contact with all or part of amino

acid residues 341, 343, 344, and 352 of CnA and amino acid

residue 123 of CnB according to Figure 1, or amino acids of

a CnA/CnB homologue that have a root mean square deviation

from the backbone atoms of said CnA and CnB amino acids of

not more than 1.5 Å.

46.   (new) The method according to claim 45,

wherein the second hydrophobic moiety comprises a hydrogen

bond donor or acceptor that can form a hydrogen bond with

all or any part of amino acid residues 341 and 352 of CnA

according to Figure 1, or amino acids of a CnA homologue

that have a root mean square deviation from the backbone

atoms of said CnA amino acids of not more than 1.5 Å.

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47. (new) The method according to any one of claims 21-24, wherein the chemical entities further comprise a linker of 8-12 Å that projects a second hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 355 and 356 of CnA according to Figure 1, or amino acids of a CnA homologue that have a root mean square deviation from the backbone atoms of said CnA amino acids of not more than 1.5 Å.

48. (new) The method according to claim 47, wherein the second hydrophobic moiety comprises a hydrogen bond donor or acceptor that can form a hydrogen bond with amino acid residue 359 of CnA according to Figure 1, or an amino acid of a CnA homologue that has a root mean square deviation from the backbone atoms of said CnA amino acid of not more than 1.5 Å.

49. (new) The method according to claim 24, wherein the hydrophobic core can make Van der Waals contact with all or part of amino acid residues 26, 46, 55, 56, 59 and 99 of FKBP12 according to Figure 1, or amino acids of a FKBP12 homologue that have a root mean square deviation

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from the backbone atoms of said FKBP12 amino acids of not
more than 1.5 Å.

50.   (new) The method according to claim 49,
wherein the hydrophobic core comprises a hydrogen bond
donor or acceptor that can form a hydrogen bond with all or
any part of FKBP12 amino acids 56 and 82 according to
Figure 1, or amino acids of a FKBP12 homologue that have a
root mean square deviation from the backbone atoms of said
FKBP12 amino acids of not more than 1.5 Å.